

Supporting Information

Mechanistic insight into the electron attachment process to guanosine in the presence of arginine

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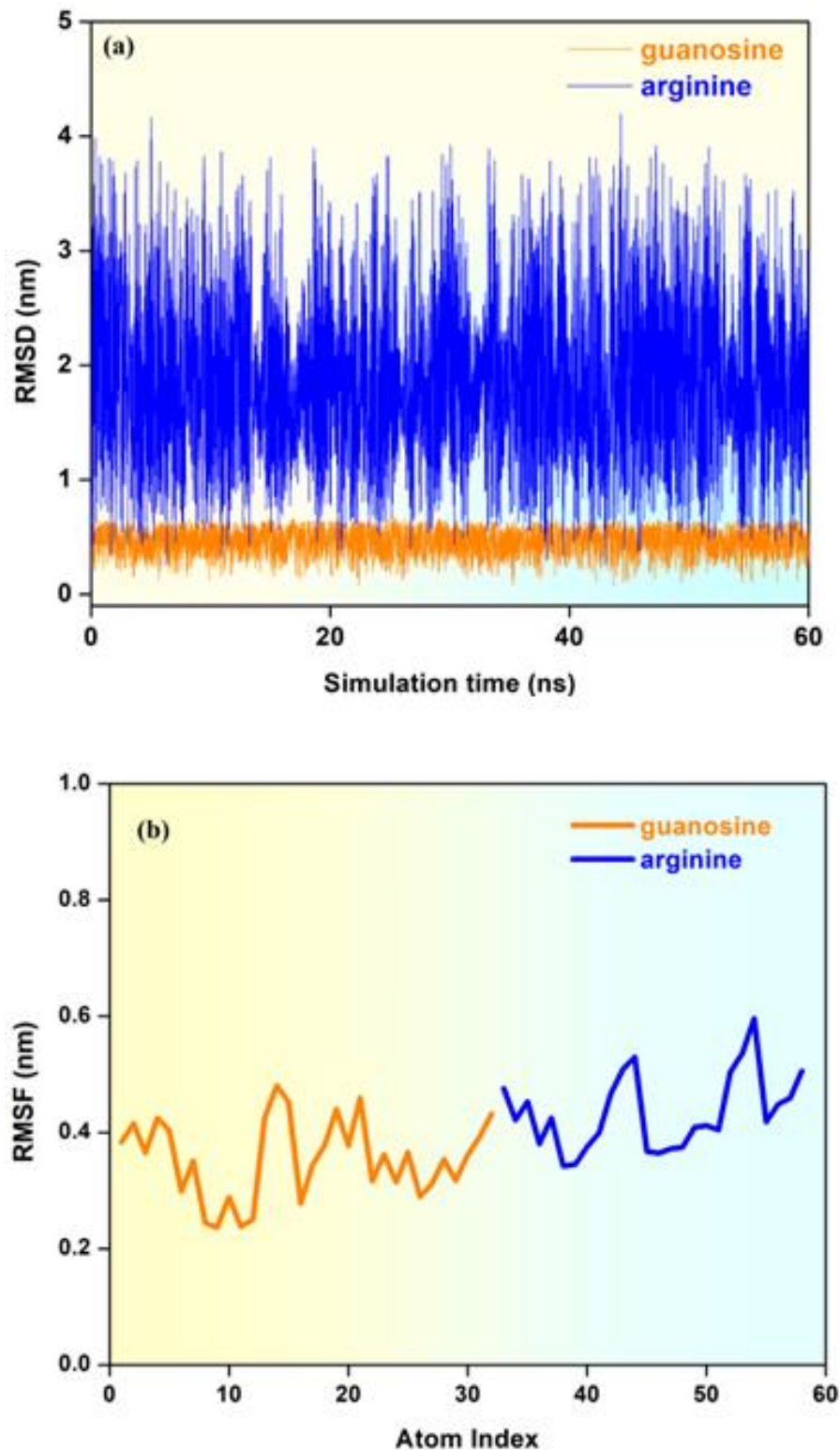


Figure S1: Root mean square deviation (RMSD) (nm) vs. simulation time for guanosine, and (b) root mean square fluctuation (RMSF) (nm) vs. atom index for guanosine and arginine.

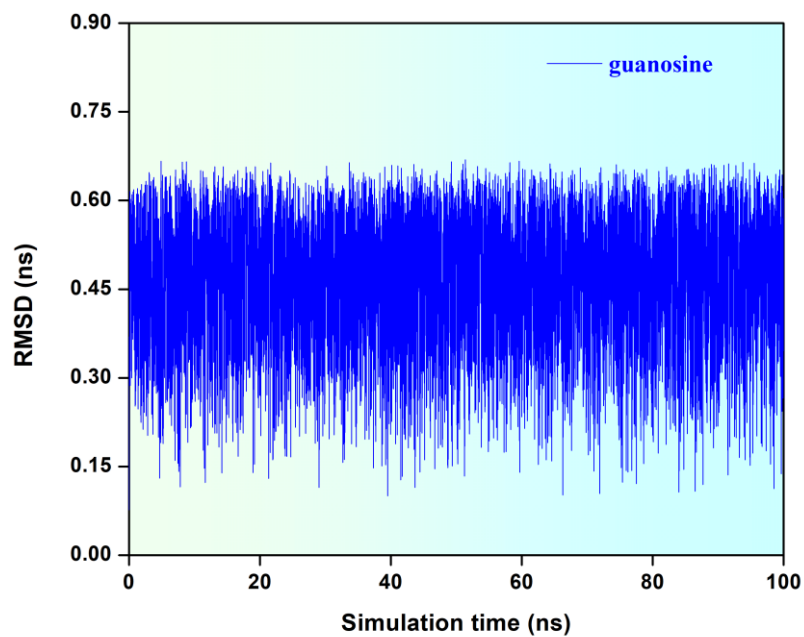


Figure S2: RMSD (nm) vs. Time (ns) for guanosine.

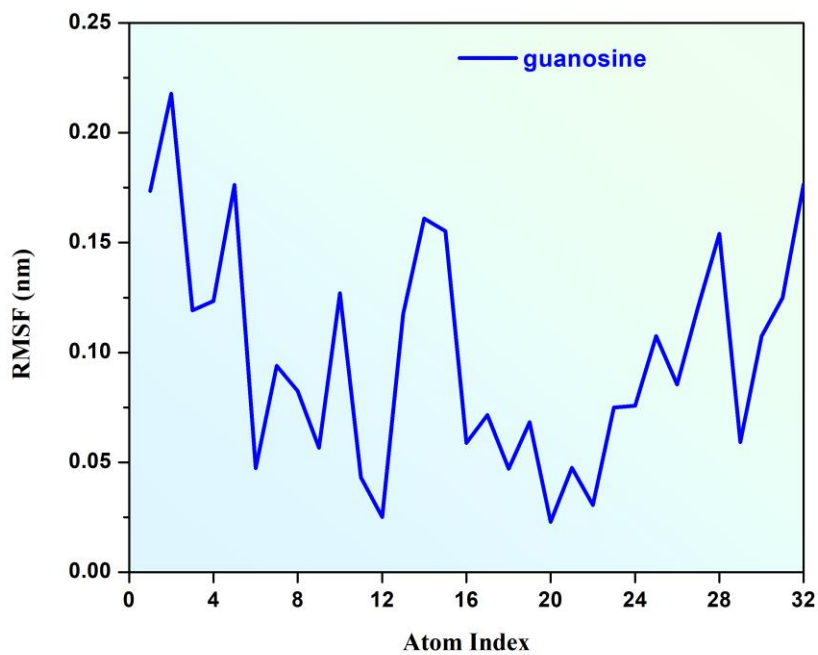


Figure S3: RMSF (nm) vs. Number of atoms of guanosine.

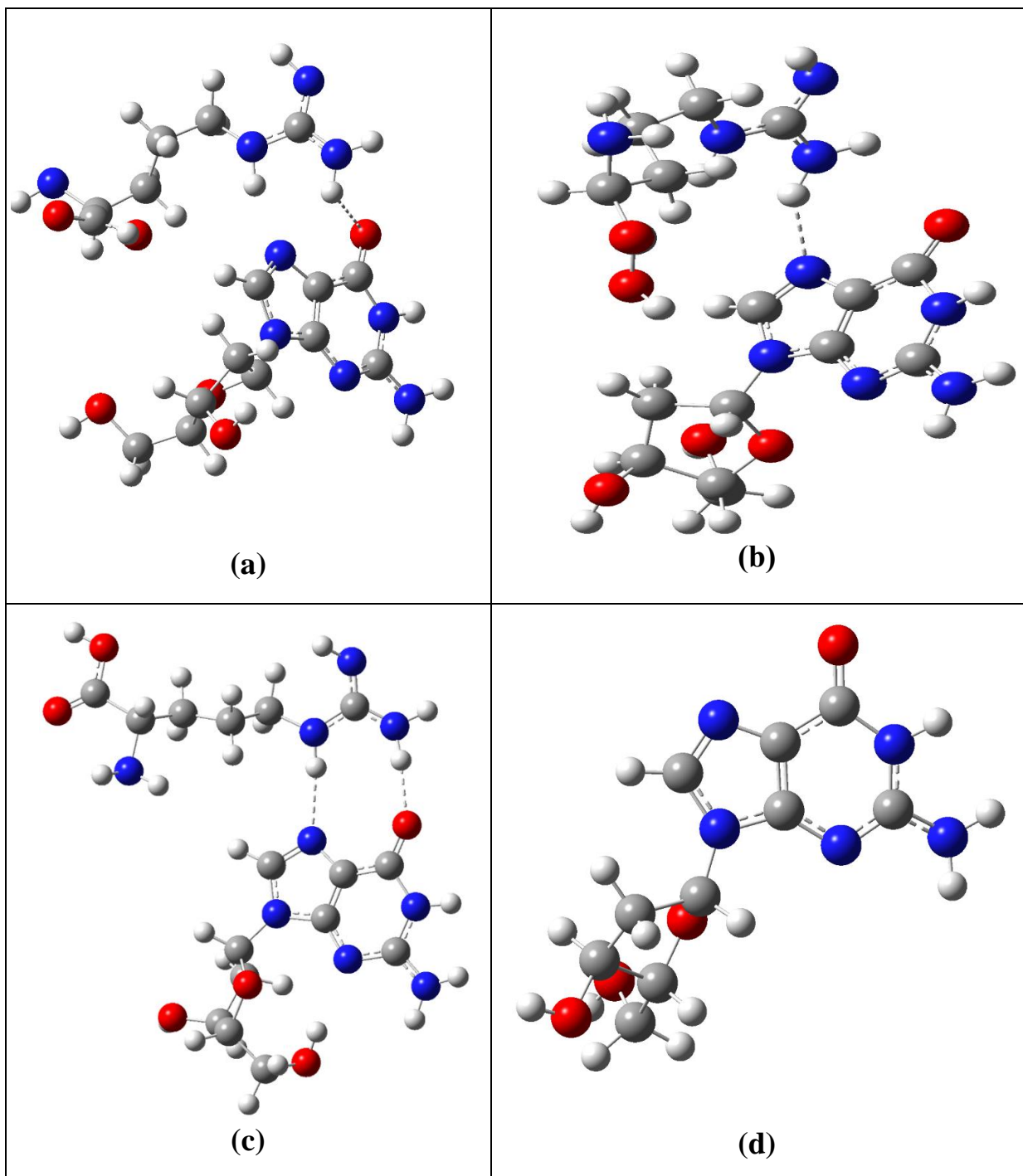


Figure S4: The frames taken from the MD simulations (a) arg-guanosine after 14 ns having one intermolecular H-bonds (1-H=O1-H1), (b) arg-guanosine after 17 ns having one intermolecular H-bonds (1-H=N3-H1), (c) arg-guanosine after 52 ns having two intermolecular H-bonds (2-H=N3-H2, O1-H1), and (d) guanosine after 100 ns (excluded surrounding water molecules).

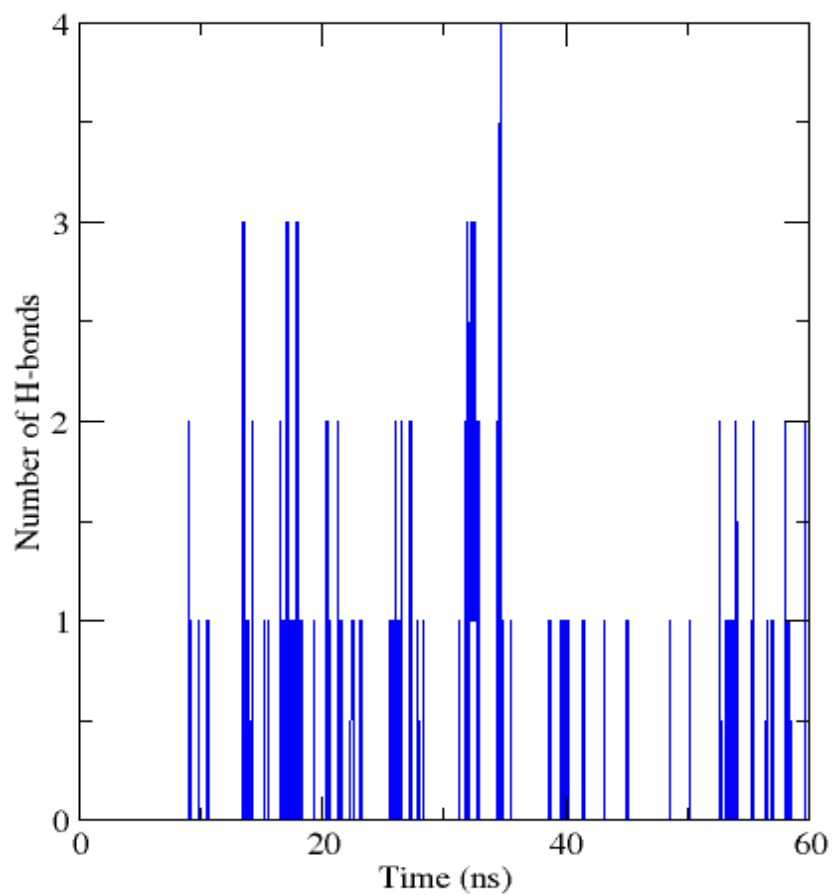


Figure S5: The number of hydrogen bonds (H-bonds) between arginine and guanosine in the MD simulations is up to 60 ns.

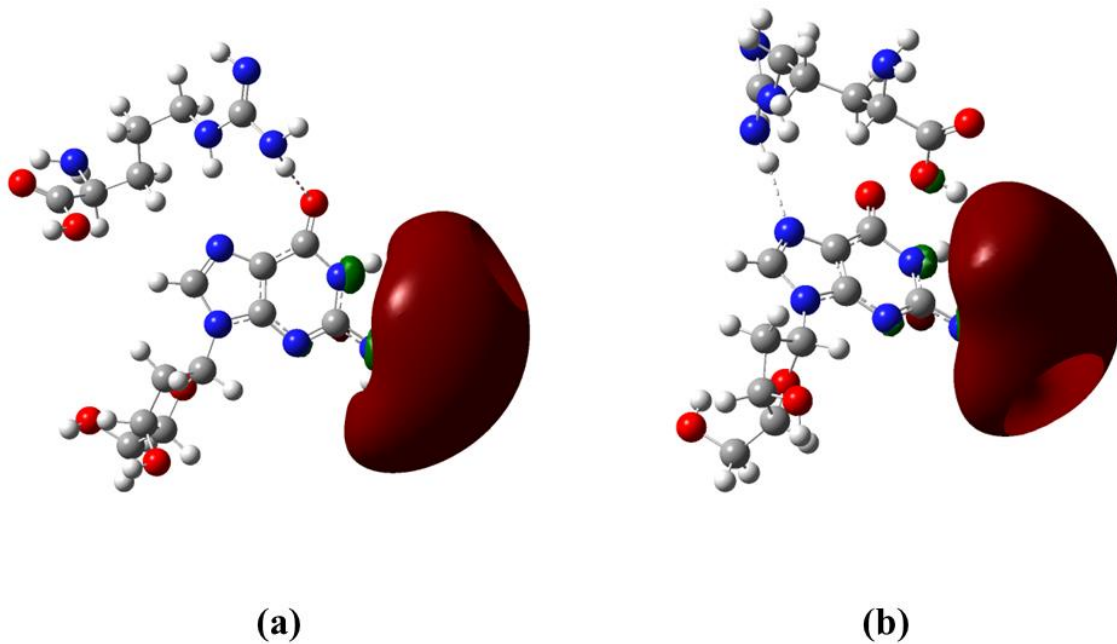


Figure S6: Singly occupied molecular orbitals (SOMOs) of (a) arg-guanosine (1-H=O1-H1) and (b) arg-guanosine (1-H=N3-H1) using MP2//B3LYP/6-311++G(d,p) level of theory.

Table S1: The VAE and VDE values for the molecules were computed using the MP2/6-311++G(d,p) level of theory. (All values are in eV).

Method	MP2/6-311++G(d,p)	
QM/MM optimized geometries	VAE	VDE
arg-guanosine (1-H=O1-H1)	-0.26	-0.11
arg-guanosine (1-H=N3-H1)	-0.27	0.05
arg-guanosine (2-H=N3-H2, O1-H1)	-1.47	0.98
guanosine	-0.41	-0.35

Table S2: Charge distribution on different fragments of the molecules [from natural population analysis (NPA)] using B3LYP/6-311++G(d,p) level of theory.

QM/MM Optimization Geometry	Neutral		
	Base (Guanine)	Sugar	Arginine
arg-guanosine (1-H=O1-H1)	-0.24e	0.25e	-0.01e
arg-guanosine (1-H=N3-H1)	-0.25e	0.26e	-0.01e
arg-guanosine (2-H=N3-H2, O1-H1)	-0.21e	0.23e	-0.02e
guanosine	-0.25e	0.25e	-

Table S3: Vertical detachment energy (eV) with every 50 fs of interval for arg-guanosine (2H = N3-H2, O1-H1), guanosine using MP2/6-311++G(d,p)//B3LYP/6-31G+(d) level of theory.

Time (in fs)	arg-guanosine (VDE) (in eV)	guanosine (VDE) (in eV)
0	0.0	0.0
50	0.24	-0.33
100	0.62	-0.33
150	1.17	-0.35
200	1.31	-0.33
250	0.98	-0.35
300	0.73	-0.11
350	0.79	-0.33
400	0.98	-0.33
450	1.44	-0.30
500	1.36	-0.35
550	0.90	-0.33
600	0.73	-0.33
650	0.98	-0.33
700	1.31	-0.35
750	1.31	-0.35
800	0.87	-0.33
850	0.79	-0.35
900	0.95	-0.30
950	1.08	-0.33
1000	1.17	-0.33

Table S4: Vertical detachment energy (eV) with every 50 fs of interval for arg-guanosine (2H = N3-H2, O1-H1), guanosine using B3LYP/6-311++G(d,p)//B3LYP/6-31G+(d) level of theory.

Time (in fs)	arg-guanosine (VDE) (in eV)	guanosine (VDE) (in eV)
0	0.0	0.0
50	1.01	0.22
100	1.33	0.22
150	1.82	0.22
200	1.96	0.24
250	1.69	0.24
300	1.42	0.27
350	1.47	0.24
400	1.69	0.24
450	2.06	0.24
500	2.01	0.27
550	1.55	0.27
600	1.44	0.26
650	1.66	0.26
700	1.96	0.24
750	1.93	0.25
800	1.55	0.24
850	1.50	0.27
900	1.60	0.27
950	1.47	0.27
1000	1.85	0.24

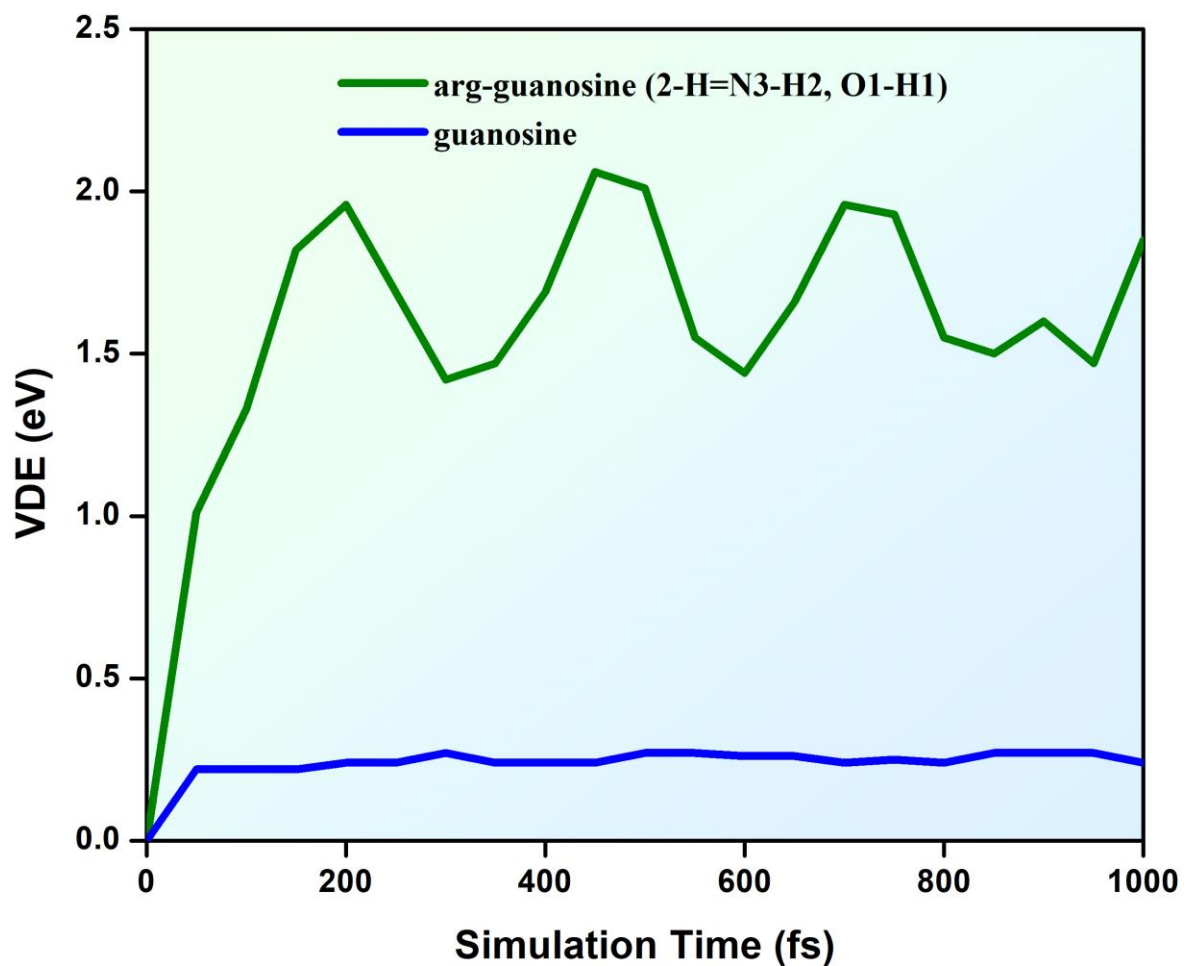


Figure S7: Vertical detachment energy (eV) vs. time (fs) (a) for arg-guanosine (2H = N3-H2, O1-H1), (b) guanosine using B3LYP/6-311++G(d,p)//B3LYP/6-31G+(d) level of theory.

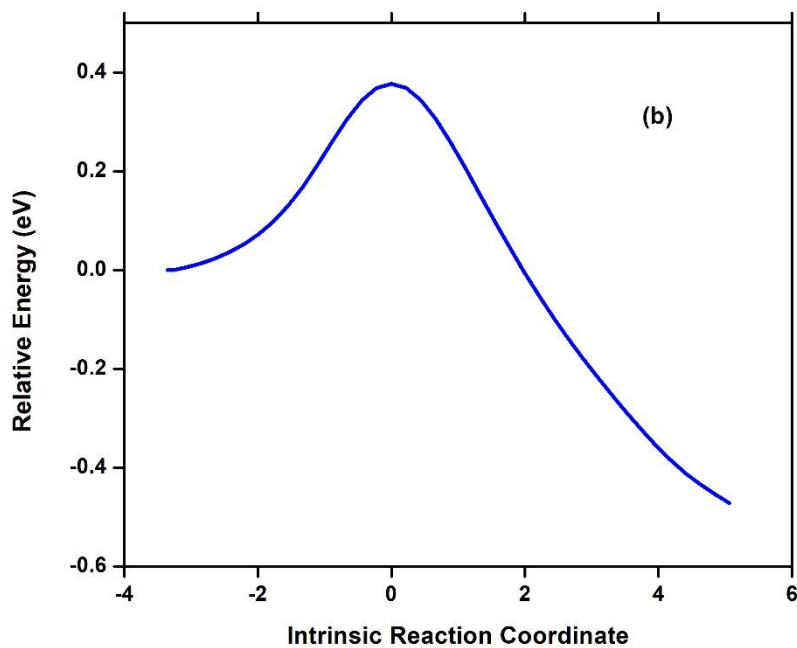
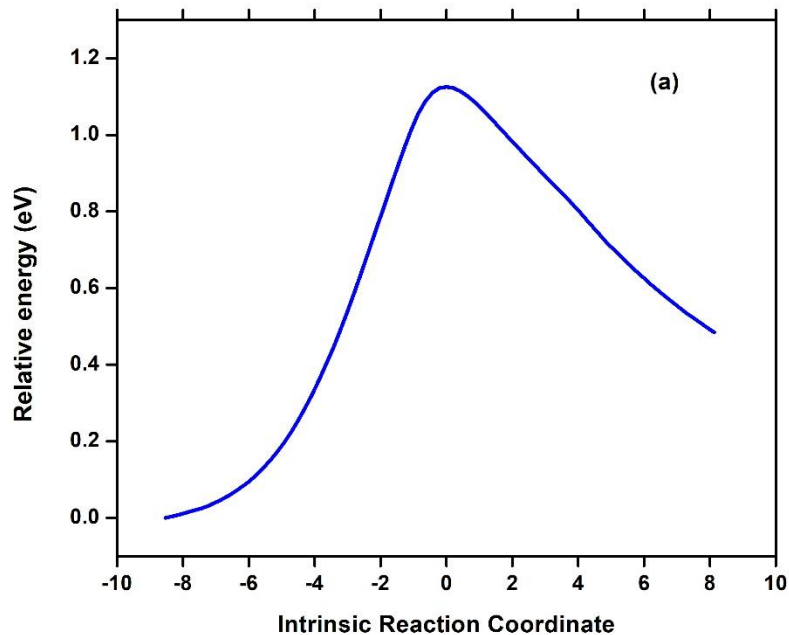


Figure S8: The intrinsic reaction coordinate (IRC) curves (a) guanosine and (b) arg-guanosine ($2H = N3-H2, O1-H1$) using B3LYP/6-311++G(d,p) level of theory for high layer and UFF for low layer surrounding water.